Finite-size instabilities in nuclear energy density functionals : finite nuclei

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Self-consistent Mean Field approaches

The nuclear EDF

The energy of the atomic nucleus is postulated as a functional

$$\mathcal{E} = \mathcal{E}_{\rm kin}(\rho) + \mathcal{E}_{\rm Sk}(\rho) + \mathcal{E}_{\rm coul}(\rho) + \mathcal{E}_{\rm pairing}(\rho,\kappa,\kappa^*) + \mathcal{E}_{\rm corr}(\rho)$$

it depends on one-body density matrix ρ and the pair tensor κ

$$\begin{split} \rho_{ij} &= \langle \Phi_0 | c_j^\dagger c_i | \Phi_0 \rangle \,, \\ \kappa_{ij} &= \langle \Phi_0 | c_j c_i | \Phi_0 \rangle \,, \\ \kappa_{ij}^* &= \langle \Phi_0 | c_i^\dagger c_j^\dagger | \Phi_0 \rangle \,. \end{split}$$

where $|\Phi_0\rangle$ is the quasi-particle vacuum

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What is in the $\mathcal{E}_{Sk}(\rho)$ box ?

 \mathcal{E}_{Sk} ? Take Hartree-Fock expectation value

$$\mathcal{E}_{\rm Sk} = \frac{1}{2} \sum_{i,j=1}^{A} \langle ij | \bar{v}^{\rm central} + \bar{v}^{\rm LS} + \bar{v}^{\rm tensor} | ij \rangle$$

of effective zero-range interaction containing a central, spin-orbit and tensor part

The central, spin-orbit, and tensor Skyrme force

$$\begin{split} v^{\text{central}} &= \left[t_0 \left(1 + x_0 \hat{P}_{\sigma} \right) + \frac{1}{6} t_3 \left(1 + x_3 \hat{P}_{\sigma} \right) \rho^{\alpha} \right] \delta(\mathbf{r} - \mathbf{r}') \\ &+ \frac{1}{2} t_1 \left(1 + x_1 \hat{P}_{\sigma} \right) \left[\hat{\mathbf{k}}'^2 \ \delta(\mathbf{r} - \mathbf{r}') + \delta(\mathbf{r} - \mathbf{r}') \ \hat{\mathbf{k}}^2 \right] \\ &+ t_2 \left(1 + x_2 \hat{P}_{\sigma} \right) \hat{\mathbf{k}}'^* \\ \delta(\mathbf{r} - \mathbf{r}') \ \hat{\mathbf{k}} \\ v^{\text{LS}} &= i W_0 \left(\hat{\sigma}_1 + \hat{\sigma}_2 \right) \cdot \hat{\mathbf{k}}'^* \\ v^{\text{tensor}} &= \frac{t_e}{2} \left\{ \left[3(\sigma_1 \cdot \mathbf{k}')(\sigma_2 \cdot \mathbf{k}') - (\sigma_1 \cdot \sigma_2) \mathbf{k}'^2 \right] \delta(\mathbf{r}) + hc \right\} \\ &+ \frac{t_o}{2} \left\{ 3(\sigma_1 \cdot \mathbf{k}') \delta(\mathbf{r})(\sigma_2 \cdot \mathbf{k}) - (\sigma_1 \cdot \sigma_2) \mathbf{k}' \cdot \delta(\mathbf{r}) \mathbf{k} + hc \right\} \end{split}$$

Introduction 00000 The Skyrme ED

From the force to the energy density functional

$$\begin{split} \mathcal{E}_{\mathrm{Sk}} &= \frac{1}{2} \sum_{i,j=1}^{A} \langle ij | \bar{v}^{\mathrm{central}} + \bar{v}^{\mathrm{LS}} + \bar{v}^{\mathrm{tensor}} | ij \rangle \\ &= \int \mathrm{d}^{3} r \sum_{t=0,1} \left\{ C_{t}^{\rho} [\rho_{0}] \rho_{t}^{2} + C_{t}^{s} [\rho_{0}] \mathbf{s}_{t}^{2} + C_{t}^{\Delta\rho} \rho_{t} \Delta\rho_{t} + C_{t}^{\nabla s} (\nabla \cdot \mathbf{s}_{t})^{2} + C_{t}^{\Delta s} \mathbf{s}_{t} \cdot \Delta \mathbf{s}_{t} \\ &+ C_{t}^{T} \left(\mathbf{s}_{t} \cdot \mathbf{T}_{t} - \sum_{\mu, \nu = x, y, z} J_{t, \mu\nu} J_{t, \mu\nu} \right) + + C_{t}^{\nabla \cdot J} (\rho_{t} \nabla \cdot \mathbf{J}_{t} + \mathbf{s}_{t} \cdot \nabla \times \mathbf{j}_{t}) \\ &+ C_{t}^{F} \left[\mathbf{s}_{t} \cdot \mathbf{F}_{t} - \frac{1}{2} \left(\sum_{\mu = x, y, z} J_{t, \mu\mu} \right)^{2} - \frac{1}{2} \sum_{\mu, \nu = x, y, z} J_{t, \mu\nu} J_{t, \nu\mu} \right] + C_{t}^{\tau} (\rho_{t} \tau_{t} - \mathbf{j}_{t}^{2}) \right\} \end{split}$$

■ The coupling constants are a function of the *t_i* and *x_i* coefficients in the Skyrme force

$$\begin{split} \rho_{q}(\mathbf{r}) &= \rho_{q}(\mathbf{r}, \mathbf{r}') \big|_{\mathbf{r}=\mathbf{r}'}, & \tau_{q}(\mathbf{r}) = \nabla \cdot \nabla' \left. \rho_{q}(\mathbf{r}, \mathbf{r}') \right|_{\mathbf{r}=\mathbf{r}'}, \\ J_{q,\mu\nu}(\mathbf{r}) &= -\frac{i}{2} \left(\nabla_{\mu} - \nabla'_{\mu} \right) s_{q,\nu}(\mathbf{r}, \mathbf{r}') \big|_{\mathbf{r}=\mathbf{r}'}, & \mathbf{j}_{q}(\mathbf{r}) = \frac{1}{2i} \left(\nabla - \nabla' \right) \left. \rho_{q}(\mathbf{r}, \mathbf{r}') \right|_{\mathbf{r}=\mathbf{r}'}, \\ \mathbf{s}_{q}(\mathbf{r}) &= \mathbf{s}_{q}(\mathbf{r}, \mathbf{r}') \big|_{\mathbf{r}=\mathbf{r}'}, & \mathbf{T}_{q}(\mathbf{r}) = \nabla \cdot \nabla' \left. \mathbf{s}_{q}(\mathbf{r}, \mathbf{r}') \right|_{\mathbf{r}=\mathbf{r}'}, \\ \mathbf{F}_{q}(\mathbf{r}) &= \frac{1}{2} \sum_{\mu,\nu=x,y,z} \left(\nabla_{\mu} \nabla'_{\nu} + \nabla'_{\mu} \nabla_{\nu} \right) s_{q,\nu}(\mathbf{r}, \mathbf{r}') \big|_{\mathbf{r}=\mathbf{r}'}. \end{split}$$

From the force to the energy density functional

$$\begin{split} \mathcal{E}_{\mathrm{Sk}} &= \frac{1}{2} \sum_{i,j=1}^{A} \langle ij | \bar{v}^{\mathrm{central}} + \bar{v}^{\mathrm{LS}} + \bar{v}^{\mathrm{tensor}} | ij \rangle \\ &= \int \mathrm{d}^{3} r \sum_{t=0,1} \left\{ C_{t}^{\rho} [\rho_{0}] \rho_{t}^{2} + C_{t}^{s} [\rho_{0}] \mathbf{s}_{t}^{2} + C_{t}^{\Delta \rho} \rho_{t} \Delta \rho_{t} + C_{t}^{\nabla s} (\nabla \cdot \mathbf{s}_{t})^{2} + C_{t}^{\Delta s} \mathbf{s}_{t} \cdot \Delta \mathbf{s}_{t} \\ &+ C_{t}^{T} \left(\mathbf{s}_{t} \cdot \mathbf{T}_{t} - \sum_{\mu,\nu=x,y,z} J_{t,\mu\nu} J_{t,\mu\nu} \right) + C_{t}^{\nabla \cdot J} (\rho_{t} \nabla \cdot \mathbf{J}_{t} + \mathbf{s}_{t} \cdot \nabla \times \mathbf{j}_{t}) \\ &+ C_{t}^{F} \left[\mathbf{s}_{t} \cdot \mathbf{F}_{t} - \frac{1}{2} \left(\sum_{\mu=x,y,z} J_{t,\mu\mu} \right)^{2} - \frac{1}{2} \sum_{\mu,\nu=x,y,z} J_{t,\mu\nu} J_{t,\nu\mu} \right] + C_{t}^{\tau} (\rho_{t} \tau_{t} - \mathbf{j}_{t}^{2}) \right\} \end{split}$$

- The coupling constants are a function of the t_i and x_i coefficients in the Skyrme force
- the EDF is a function of densities, currents and tensors. Some transform even under time reversal, other transform odd under time reversal.

$$\rho_q^T(\mathbf{r}) = \rho(\mathbf{r})$$

$$\mathbf{s}_q^T(\mathbf{r}) = -\mathbf{s}_q(\mathbf{r})$$

How it started : Instabilities/divergencies in cr8

- Systematic divergencies in cr8 found for several TIJ parameterizations after implementation of the tensor terms
- The calculation stops because the total energy diverges or the total energy becomes positive.

The culprits ?

$$\begin{split} \mathcal{E}_{\mathrm{Sk}} &= \int \mathrm{d}^3 r \sum_{t=0,1} \left\{ C_t^{\rho} \rho_t^2 + C_t^{\mathrm{s}} \mathbf{s}_t^2 + C_t^{\Delta \rho} \rho_t \Delta \rho_t + C_t^{\Delta \mathrm{s}} \mathbf{s}_t \cdot \Delta \mathbf{s}_t \\ &+ C_t^T \left(\mathbf{s}_t \cdot \mathbf{T}_t - \sum_{\mu,\nu=x,y,z} J_{t,\mu\nu} J_{t,\mu\nu} \right) + C_t^\tau \left(\rho_t \tau_t - \mathbf{j}_t^2 \right) \\ &+ C_t^{\nabla \cdot J} (\rho_t \nabla \cdot \mathbf{J}_t + \mathbf{s}_t \cdot \nabla \times \mathbf{j}_t) + C_t^{\nabla \mathrm{s}} (\nabla \cdot \mathbf{s}_t)^2 \\ &+ C_t^F \left[\mathbf{s}_t \cdot \mathbf{F}_t - \frac{1}{2} \left(\sum_{\mu=x,y,z} J_{t,\mu\mu} \right)^2 - \frac{1}{2} \sum_{\mu,\nu=x,y,z} J_{t,\mu\nu} J_{t,\nu\mu} \right] \right\} \end{split}$$

season ? finite-size instabilities ?

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Some technical details

Calculation details

- HFB + LN (+ self-consistent cranking)
- In pairing channel : surface density-dependent δ interaction with 5 MeV cutoff above and below the Fermi level and V=-1250 MeV fm⁻³
- cr8 and evb8 :
 - parity and z-signature
 - 3D Cartesian mesh
 - imaginary time-step method

$$|\tilde{\phi}_k^{(i)}
angle = 1 - \frac{dt}{\hbar}h^{(i)}|\phi_k^{(i-1)}$$

dt ~
$$dx^2$$
 (for $dx = 0.8$ fm,
 $dt = 0.012 \ 10^{-22}$ s)



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Introduction Self-Consistent Mean

Systematic divergencies

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Finite-size instabilities ?

Finite-size instabilities?

What are they ?

- They are associated with strong derivative terms in the Skyrme EDF : $\rho_t \Delta \rho_t$, $\mathbf{s} \cdot \Delta \mathbf{s}$, and $(\nabla \cdot \mathbf{s})^2$
- They cause systematic non-convergence in SCMF calculations
- They can be studied with linear response theory in INM : calculate the response of INM to perturbations of the density.
 - ∞ wavelength \rightarrow cfr. Landau parameters
 - finite wavelength \rightarrow finite-size instability

Finite-size instability caused by $\rho_1 \Delta \rho_1$





Toy model : Take the SLy5 parameterisation and vary $C_1^{\Delta\rho}$. Compare RPA in INM and results for finite nucleus (¹³²Sn)



(A. Pastore et al., arXiv:1110.6377 (2011))

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Toy model : Take the SLy5 parameterisation and vary $C_1^{\Delta\rho}$. Compare RPA in INM and results for finite nucleus (¹³²Sn)



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The $\rho_1 \Delta \rho_1$ term favours strong oscillations in the proton and neutron density

Conclusion

Finite-size instabilities ?

How important are these $(\nabla \cdot \mathbf{s})^2$ and $\mathbf{s} \cdot \Delta \mathbf{s}$ terms ?

SD band in ¹⁹⁴Hg



- \Box $C_t^{\Delta s}$ values chosen close to limit of stability to obtain maximal effect
- Small, sign-dependent effect on $\mathcal{J}^{(2)}$
- Similar for $C_t^{\nabla s}$

Thus .

Small terms that can be very annoying...

Force vs functional

Force vs functional



(M. Bender et al., PRC 79, 044319 (2009))

Why not adopt the EDF approach and put these terms to zero ?

 \rightarrow anomalies appear in the PNR deformation energy surface when you take enough discretization points of the integral over the gauge angle

Solutions ?

- Regularization scheme (eliminate spurious terms). This requires forces with $\alpha = 1$
- Use an effective strong + Coulomb interaction with all direct, exchange and pairing terms

Force vs functional

Force vs functional



- We cannot switch off these small derivative terms
- Need for stable forces !
- Especially difficult for time-odd (∇ ⋅ s)² and s ⋅ ∆s as they are zero during the fitting procedure

Our goal is two-fold :

- Define a save interval
- Understand what is going on at the instability
- Establish the link between finite nuclei and INM

Why not adopt the EDF approach and put these terms to zero ?

 \rightarrow anomalies appear in the PNR deformation energy surface when you take enough discretization points of the integral over the gauge angle

Solutions ?

Regularization scheme (eliminate spurious terms). This requires forces with $\alpha = 1$

Use an effective strong + Coulomb interaction with all direct, exchange and pairing terms

First, start from what we know : $\rho_1 \Delta \rho_1$



⁽A. Pastore et al., arXiv:1110.6377 (2011))

Scan of $C_1^{\Delta \rho}$ in 3D codes

 \blacksquare ²⁰⁸Pb with SLy5 interaction and evb8



\Rightarrow Non-convergence at positive and negative side

Finite-size instabilities in finite nuclei

Conclusion

Evolution of ρ_1 at $C_1^{\Delta \rho} = 40$



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Finite-size instabilities in finite nuclei

Conclusion

Evolution of ho_0 at $C_1^{\Delta ho} = 40$



Linear Response Theory : from infinite nuclear matter to finite nuclei

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Finite-size instabilities in finite nuclei

 $\rho_1 \Delta \rho_1$

$\rho_t, \Delta \rho_t \text{ and } \rho_t \Delta \rho_t \text{ at } C_1^{\Delta \rho} = 40$



iter=70



What is seen in infinite nuclear matter

(with the SLy5 parameterization)



A. Pastore, private communication

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Finite-size instabilities in finite nuclei

Now, proceed to : $\mathbf{s}_0 \Delta \mathbf{s}_0$



Vary $C_0^{\Delta s}$ ($C_1^{\Delta s} = C_t^{\nabla s} = 0$) for $J_z = 54$ in ¹⁹⁴Hg with T22 parameterization

Outside this domain, the calculation diverges !

$$\square C_0^{\Delta s} > 0$$

- steep downward slope of $E(s_0\Delta s_0)$
- strong change in spin-polarization

 $\blacksquare C_0^{\Delta s} < 0$

no strong variation

Empirical limits :

 $C_t^{\Delta s} = [-24:36] \text{ MeV fm}^5$

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- ¹⁹⁴Hg at Jz=54 with T22 interaction and cr8
- dx=0.8 fm, dt=0.012 10⁻²² s
- For $C_t^{\Delta s} = 0$ MeV fm⁵, the spins are aligned to the rotation axis at J_z =54

Finite-size instabilities in finite nuclei

Evolution of \mathbf{s}_0 at $C_0^{\Delta s} = 40 \text{ MeV fm}^5$



iter=10





Linear Response Theory : from infinite nuclear matter to finite nuclei

\mathbf{s}_0 , $\Delta \mathbf{s}_0$ and $\mathbf{s}_0 \cdot \Delta \mathbf{s}_0$ at $C_0^{\Delta s} = 40 \text{ MeV fm}^5$





- At 150 iterations
- Negative coupling constant : E(s₀Δs₀) becomes strongly negative

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What is seen in infinite nuclear matter

(with the T22 parameterization)



A. Pastore, private communication

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How about $(\boldsymbol{\nabla} \cdot \mathbf{s}_0)^2$



Vary $C_0^{\nabla s}$ ($C_t^{\Delta s} = C_1^{\nabla s} = 0$) for $J_z = 54$ in ¹⁹⁴Hg with T22 parameterization

Outside this domain, the calculation diverges !

Empirical limits :

$$C_0^{\nabla s} = [-56:92] \text{ MeV fm}^5$$

 $C_1^{\nabla s} = [-48:96] \text{ MeV fm}^5$

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The spin density \mathbf{s}_0 and $\mathbf{\nabla} \cdot \mathbf{s}_0$ at $C_0^{\nabla s} = -60 \text{ MeV fm}^5$

At 10 iterations



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The spin density \mathbf{s}_0 and $\mathbf{\nabla} \cdot \mathbf{s}_0$ at $C_0^{\nabla s} = -60 \text{ MeV fm}^5$

At 200 iterations



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The spin density \mathbf{s}_0 and $\nabla \cdot \mathbf{s}_0$ at $C_0^{\nabla s} = -60 \text{ MeV fm}^5$

At 400 iterations



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The spin density \mathbf{s}_0 and $\nabla \cdot \mathbf{s}_0$ at $C_0^{\nabla s} = -60 \text{ MeV fm}^5$

At 550 iterations



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What is seen in infinite nuclear matter

(with the T22 parameterization)



A. Pastore, private communication

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The "negative side" of the coupling constants

What about the "negative side" ?



- The instability at neg. values of C are not observed in INM
- Instability or just non-convergence ?



The "negative side" of the coupling constants

What about the "negative side" ? Divergence or instability ?



- Calculation normally stops around 200 iterations for $C_1^{\Delta\rho} = -260 \text{ MeV fm}^5$
- Beyond 200 iteration, it becomes "metastable" with very bad convergence of the s.p. levels
- dx=0.8 fm, dt=0.012 10⁻²² s



The "negative side" of the coupling constants

What happens with ho_0 for $C_1^{\Delta ho} = -260 \text{ MeV fm}^5$

(Loading movie ...)

- Calculation for ²⁰⁸ Pb with dx=0.8 fm, dt=0.012 10⁻²² s
- Isosurface of ρ_0 at 95% of $\rho_{0,max}$
- Nucleus essentially "falls apart" (respecting the symmetries of the code, hence octahedral shape)



Linear Response Theory : from infinite nuclear matter to finite nuclei

Conclusion

The "negative side" of the coupling constants

What happens with
$$ho_1$$
 for $C_1^{\Delta
ho} = -260 \text{ MeV fm}^5$

(Loading movie ...)

- Calculation for ²⁰⁸ Pb with dx=0.8 fm, dt=0.012 10⁻²² s
- Isosurface of ρ_1 at 60% of $\rho_{1,max}$



Linear Response Theory : from infinite nuclear matter to finite nuclei

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Disclaimer : The exact value of the coupling constant where non-convergence first occurs is sensitive to the numerics of the problem (basis or mesh, damping, etc), to the mass number of the nucleus, to the other parameters, ...



HFODD converges (?) for $C_1^{\Delta s} = 40$ MeV fm⁵ and $C_1^{\Delta s} < -24$ MeV fm⁵, which is unstable with cr8

Some numerics

Test for 208 Pb, with dx=0.8 fm (up to 2000 iterations) (dt= time step in the imaginary time-step method)

	$C_1^{\Delta \rho}$ [MeV fm ⁵]				
$dt [10^{-22} s]$	-260	-280	-300	-320	
0.009	\checkmark	\checkmark	\checkmark	\checkmark	
0.010	\checkmark	\checkmark	\checkmark	X	
0.011	\checkmark	\checkmark	Х	X	
0.012	Х	Х	Х	X	

- Calculation with dt=0.011 10^{-22} s starting from "metastable" result for dt=0.012 10^{-22} s converges ($C_1^{\Delta\rho}$ =-260)
- Calculation with dt=0.012 10^{-22} s starting from "converged" result for dt=0.011 10^{-22} s diverges ($C_1^{\Delta\rho}$ =-260)
- Calculation with dt=0.011 10^{-22} s starting from dt=0.011 10^{-22} s $(C_1^{\Delta\rho}$ =-260) with ndiag = 1 converges (ndiag=1 : diagonalization before iterations start)

Play with damping

nxmu=10 ($W^{(n+1)} = nxmu/100 * W^{(n+1)} + (1 - nxmu/100) * W^{(n)}$)

	$C_1^{\Delta \rho}$ [MeV fm ⁵]				
dt [10 ⁻²² s]	-260	-300	-340	-380	-420
0.006	\checkmark	\checkmark	\checkmark	\checkmark	
0.008	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark
0.010	\checkmark	\checkmark	\checkmark	\checkmark	Х
0.012	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark

nxmu=20

	$C_1^{\Delta \rho}$ [MeV fm ⁵]				
dt [10 ⁻²² s]	-260	-300	-340	-380	-420
0.006	\checkmark	\checkmark	\checkmark	\checkmark	
0.008	\checkmark	\checkmark	\checkmark	Х	Х
0.010	\checkmark	\checkmark	\checkmark	Х	Х
0.012	\checkmark	Х	Х	Х	Х

nxmu=30

	$C_1^{\Delta \rho}$ [MeV fm ⁵]				
dt [10 ⁻²² s]	-260	-300	-340	-380	-420
0.006	\checkmark	\checkmark	\checkmark	\checkmark	
0.008	\checkmark	\checkmark	Х	Х	Х
0.010	X	Х	Х	Х	Х
0.012	X	Х	Х	Х	Х

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Play with damping

nxmu=10 (damping parameter)

	$C_1^{\Delta \rho}$ [MeV fm ⁵]				
dt [10 ⁻²² s]	-260	-300	-340	-380	-420
0.006	\checkmark	\checkmark	\checkmark	\checkmark	
0.008	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark
0.010	\checkmark	\checkmark	\checkmark	\checkmark	Х
0.012	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark

nxmu=25 : start calculation from fully "converged" calculation with nxmu=10

	$C_1^{\Delta \rho}$ [MeV fm ⁵]				
dt [10 ⁻²² s]	-260	-300	-340	-380	-420
0.006	\checkmark	\checkmark	\checkmark	\checkmark	
0.008	\checkmark	\checkmark	\checkmark	\checkmark	Х
0.010	\checkmark	Х	Х	Х	Х
0.012	X	Х	Х	Х	Х

 \Rightarrow It seems as if the nxmu= 10 calculation is "fake" converged. Diminishing the time step is also some sort of damping.

Some conclusions and questions

- We found finite-size instabilities for the $(\nabla \cdot \mathbf{s})^2$ and the $\mathbf{s}\Delta\mathbf{s}$ terms for all TIJ. We have scanned the range of their respective coupling constants where these terms remain stable.
- **We** have studied the $\rho_1 \Delta \rho_1$, the **s** Δ **s**, and the $(\nabla \cdot \mathbf{s})^2$ in detail.
- Studies in infinite nuclear matter confirm the "positive" end of the safe range but not the negative side. How to study the negative side ? Can it be done with INM ?

Disclaimer : The exact value of the coupling constant where non-convergence first occurs is sensitive to the numerics of the problem (basis or mesh, damping, etc), to the mass number of the nucleus, to the other parameters, ...

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Thanks for your attention !